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Title: Initial beta-tin stress-strain calibration

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1 Introduction

This is a strength model calibration of the Preston-Tonks-Wallace (PTW) model of plastic deformation for extreme loading conditions [1] using a multi-phase equation of state for tin, but for the nonce limited to the β phase.

2 Shear modulus model

To model the shear modulus we use a generalized form for arbitrary densities and temperatures [2], the generalized BGP model. This shear modulus matches available data averaged over phases as a function of density. The parameters used in this case are

$$\gamma_1 = \quad 2.2, \quad q_1 = 1/3, \tag{1}$$

$$\gamma_2 = \quad -1.0, \quad q_2 = 0.7, \tag{2}$$

$$\rho_0 = \quad 7.4, \quad G(\rho_0, T = 0) = 27. \tag{3}$$

The units are grams/cm^3 for ρ and GPa for G.

This model can be compared with the shear modulus table included in the Sesame multi-phase tin EoS [3]. The two are shown in Figure 1. For the purpose of the fits, the generalized BGP shear was fit over a range of densities from six to eight grams per cm^3. The polynomial form of the fit is

$$G(\rho) = 22.0612 - 9.97669\rho + 1.43858\rho^2 \text{ GPa}. \tag{4}$$

The thermal softening uses the form $G(\rho, T) = G(\rho, 0)[1 - \beta T/T_m(\rho)]$. This fit uses $G(\rho, 0)$ from the generalized BGP form and the melt temperature $T_m(\rho)$ from the Sesame 2161 solidus melt table, along with $\beta = 0.5$ to represent the average thermal softening for any phase.

3 Calibration data

The calibration data is from Anderson *et al* [4], which includes three quasistatic (QS) compression tests and four split Hopkinson pressure bars (SHPB) at rates near 3000/s. We include one additional QS data set in our fits but it does not have a large effect on the results.

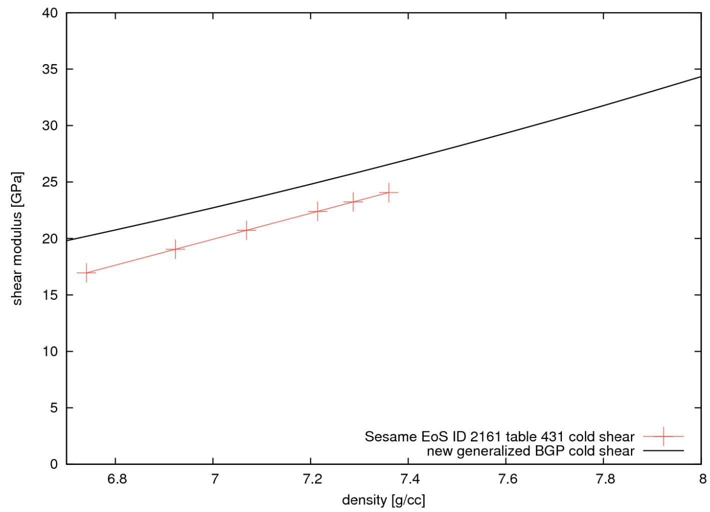

Figure 1: Comparison between Sesame 2161 shear table and the generalized BGp shear model used here.

The strain response of the low rate QS and higher rate SHPB data sets are somewhat discrepant, so we include three fits. Individual fits to the QS and SHPB data sets are included after the primary overall fit. These data sets are described in Table 1. All three fits are shown compared to two of the data sets in Figure 2.

3.1 Parameter values

The primary fit is given in Table 2, which achieves agreement with an average rms discrepancy of $< 9\%$ between the calibration data and the model. Alternate fits to subsets of the data (QS or SHPB only) achieve rms deviations on the order of 4%. A validation comparison between the calibration data, the fit result and a hydrocode output is shown for the 3000/s, 328 K data set in Figure 3.

4 Supplementary information

In the generalized BGP formulation, the parameters γ_k and q_k lead to the strange units for γ_k of ρ^{q_k}. To facilitate conversion between possibly different units, the calculations shown in the SPHB validation effort use instead $\gamma_1^3 = 10.648$ and $\gamma_2^{1/0.7} = 1$.

The mass per atom was defined to be $A/N_A = 118.71/(6.023 \cdot 10^{23})$.

Finally, we include Table 3 with separate fits to the QS and SHPB data which both obtain agreement to about 4% with their respective data sets.

Strain rate [1/s]	ψ_{min}	ψ_{max}	T [K]	C_V[J/kg/K]	Q/W	weight
3000.0	0.006	1.0	328.0	213.0	1.0	0.9742
3000.0	0.006	1.0	295.0	212.1	1.0	0.9921
3000.0	0.006	1.0	273.0	211.3	1.0	0.9895
2750.0	0.006	1.0	233.0	209.3	1.0	0.9545
0.001	0.01	1.0	253.0	-	-	0.7013
1.0	0.01	1.0	295.0	-	-	0.6714
0.001	0.01	1.0	295.0	-	-	1.4427
5.0	0.01	1.0	295.0	-	-	3.3451

Table 1: Parameters describing calibration data sets and fits. The entries with a specific heat given were treated adiabatically, while the others were treated isothermally.

Parameter	Value
θ	0.0600
p	2
s_0	0.028857
s_∞	0.000752
κ	0.1508
γ	0.00001
y_0	0.006764
y_∞	0.000120
y_1	0.0355
y_2	0.45
β	0.45

Table 2: Recommended parameter values from model calibration. Note that the parameters y_1, y_2 and β were fixed and are inherited values. Future work should include an effort to include higher strain rate shock data to inform these parameter values.

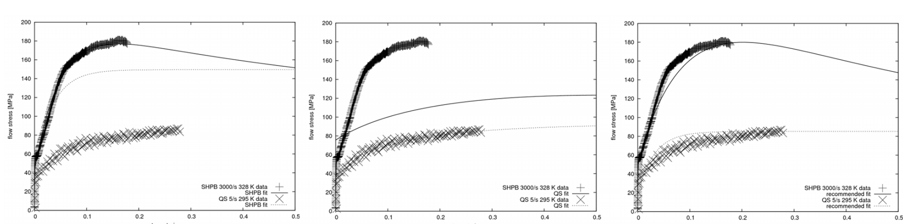

Figure 2: A comparison between the three fits. Left is the SHPB fit, center is the QS fit, and on the right is the recommended fit.

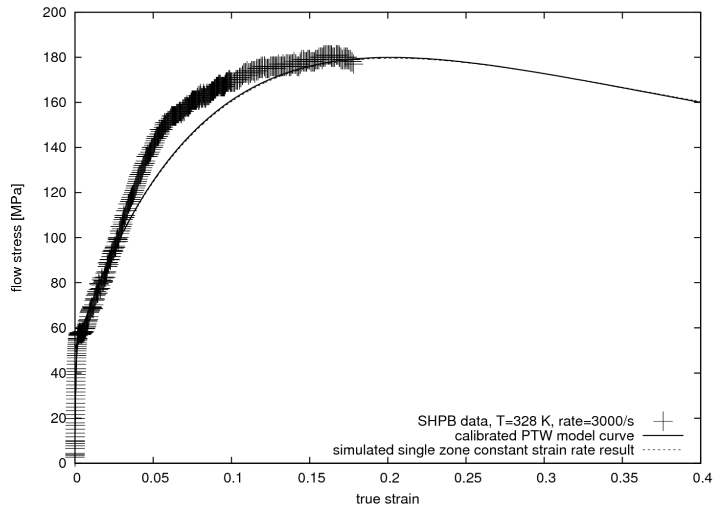

Figure 3: Calibration data, fit, and constant strain rate simulation. The simulation and the fit are nearly indistinguishable.

Parameter	QS value	SHPB value
θ	0.0105	0.09
p	4	1
s_0	0.008692	0.03538
s_∞	0.000206	0.00391
κ	0.1012	0.2256
γ	0.000001	0.00001
y_0	0.004026	0.003338
y_∞	0.000176	0.001097
y_1	0.0355	0.0355
y_2	0.45	0.45
β	0.45	0.45

Table 3: Best fits found strictly using QS or SHPB data. Neither of these fits perform well when considering all of the data.

References

[1] Dean L. Preston, Davis L. Tonks and Duane C. Wallace, *Model of plastic deformation for extreme loading conditions*, J. Appl. Phys. **93**, 211 (2003)

[2] Burakovsky *et al.*, *Generalization of the unified analytic melt-shear model to multi-phase materials: molybdenum as an example*, Crystals **2019**, 9, 86

[3] Greeff, C.W. *et al.*, *SESAME 2161: An explicit multiphase equation of state for tin*, Los Alamos National Laboratory report LA-UR-05-9414 (2005)

[4] William W. Anderson *et al.*, *Phase transition and spall behavior in β-tin*, Shock Compression of Condensed Matter 1999, 443